Pairing matrix elements and the average single-particle level density: A simple and efficient estimation method

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Bohr, Mottelson and Pines have singled out two nuclear spectroscopic properties affected strongly by nuclear pairing and possibly accessible to mean field approaches

- Moments of inertia of well and rigidly deformed even-even nuclei

- Odd-even mass differences (in well and rigidly deformed nuclei)

Using such data, we aim at providing a simple yet efficient method to determine phenomenologically the intensity of pairing correlations to be considered in these approaches

As a first step, we deal with calculations within the Hartree-Fock (with self-consistent blocking when necessary) plus pairing correlations within the simple seniority force ansatz

We are thus searching here for a safe determination of average pairing matrix elements

This approach could be considered as usual but we include here two important features absent in all previous similar works

The limitation to well and rigidly deformed nuclei is motivated by

minimizing quantal shape fluctuations, maximizing the relevance of a single mean-field wavefunction description

allowing to describe with a good approximation nuclear ground states from intrinsic states within the Bohr-Mottelson unified model (plus using the pure rotor approximation to determine the moments of inertia)

Moments of inertia are deduced from the energy of the first 2+ state in even-even nuclei as

$$J / \hbar^2 = 3 / E(2^+)$$

Odd-even three-points mass differences
of odd neutron – even proton nuclei (N,Z) for instance
are considered here and defined as

$$\delta_n^{(3)}(N,Z) = 1/2\,[2E(N,Z) - E(N+1,Z) - E(N-1,Z)]$$
$$= 1/2\,[S_n(N+1,Z) - S_n(N,Z)]$$

(where $S_n(N,Z)$ is the separaton energy of a (N,Z) nucleus)

A fit on a large enough nuclear region is akin of making
a semiclassical average

Entering some average pairing gap formulae $\Delta_q(N, Z)$ (with $q = n, p$)
and computing semiclassical estimates *
of the average sp level densities $\rho_q(e)$ for given quantal spectra

* approximated through a standard (energy) smoothing à la Strutinsky

One deduces the pairing matrix elements V_q averaged over an interval 2ω around the Fermi energy λ_q through the gap equation

$$\frac{1}{V_q} = \int_{\lambda_q - \omega}^{\lambda_q + \omega} \frac{\rho_q(e)\, de}{\sqrt{(e - \lambda_q)^2 + \Delta_q^2}}$$

with N_q standing for N or Z such that $N_q = \int_{-\infty}^{\lambda_q} \rho_q(e)\, de$

(to avoid problem with the continuum, on should restrict to nuclei not too close to the drip lines)

The average sp level density $\rho_q(e)$ is the key quantity determining the pairing intensiiesy in a given nucleus

Two important features (pertaining to this sp level density) of such a standard fitting approach currently not considered in similar microscopic calculations, are taken into account here

1) Selecting well and rigidly deformed ground states, one introduces a bias by sampling sp spectra with sp level densities at the Fermi energy systematically lower than average as noted by P. Möller and J.R. Nix, Nucl. Phys. A536 (1992) 20.

Therefore one must not use there standard fits as in A.S. Jensen and P.G. Hansen, Nucl. Phys. A431 (1984) 393. D. Madland and J.R. Nix, Nucl. Phys. A476 (1988) 1.

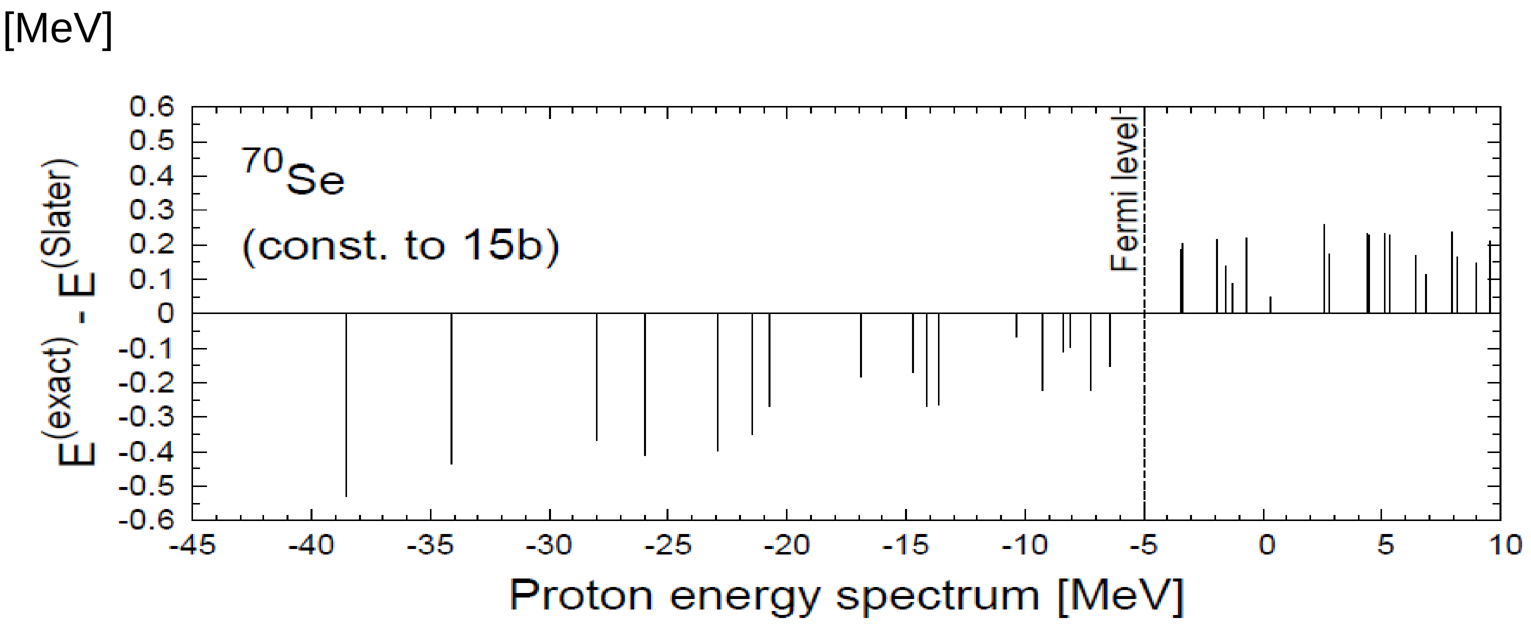
We use rather the values given by P. Möller and J.R. Nix:

$$\Delta_q(N_q) = \frac{4.8}{N_q^{1/3}} \; (\mathrm{MeV})$$

However this should be corrected for the protons due to another bias present in almost all such microscopic calculations

In most Hartree-Fock plus BCS or Hartree-Fock-Bogolyubov and in all EDF calculations one makes easier the calculation of Coulomb exchange terms by using a local Slater approximation

This as noted years ago, confirmed and explained later entails a systematic and significant spurious enhancement of the proton sp level density near the Fermi surface



J.L Le Bloas, M.-H. Koh, P. Quentin, L. Bonneau, J. Ithnin, Phys . Rev. C84 (2011) 0143310

This has been taken care of by renormalizing the Möller Nix ansatz by a factor deduced from exact microscopic Coulomb calculations as

$$\Delta_q\left(N_q\right) = X \; \frac{4.8}{N_q^{1/3}} \left(\text{MeV}\right) \text{ typically } X \text{ is of the order of } 0.8$$

$$\text{with } X = \frac{\Delta_{\text{exact}}}{\Delta_{\text{Slater}}} \text{ as obtained in quantal Hartree-Fock + BCS calculations}$$

It has been found that such a corrective factor may be evaluated with a good approximation according to the value of the average proton pair condensation energy

$$E^{p}_{cond.} = \frac{\Delta_p^2}{V_p} \quad \text{as} \quad X \approx 0.0181\, E^{p}_{cond.} + 0.781 \;\; \left(\text{where } E^{p}_{cond.} \text{ is given in MeV}\right)$$

avoiding thus to make exact Coulomb calculations for each nucleus with a very fast converging iterative process on V_p

What is the effect on the average pairing matrix elements of taking into account these effects ?

We made a test for three even-even rare earth nuclei in the A= 176-178 region: ^{176}Yb, ^{178}Yb, ^{178}Hf

We list the matrix elements with the values of G_q defined from V_q as (P. Bonche et al., Nucl. Phys. A 443 (1985) 39) :

$$V_q = G_q/11 + N_q \quad \text{giving } G_q \text{ in MeV}$$

	Jensen no Slater corr		Jensen with Slater corr		Moller-Nix no Slater corr		Moller-Nix with Slater corr	
	Vn	Vp	Vn	Vp	Vn	Vp	Vn	Vp
^{176}Yb	18.5094	17.9901	18.5094	16.9533	19.6677	19.2213	19.6677	17.9415
^{178}Yb	18.1356	17.7228	18.1356	16.6617	19.5874	19.0755	19.5874	17.8524
^{178}Hf	18.9891	18.2517	18.9891	17.2806	19.7145	19.0236	19.7145	17.9612

For neutron matrix elements

Of course the Slater approx. correction does not affect them

Going from Möller-Nix to Jensen gaps they decrease by 5-7%

For proton matrix elements

Going from Möller Nix to Jensen gaps they decrease by 6-9%

Omitting the Slater approx. correction they increase by 6-7%

Combining both changes the values vary by less than 2%

Results for the moments of inertia of well and rigidly deformed even-even nuclei

They are calculated à la Inglis-Belyaev from Hartree-Fock plus BCS (with seniority force) solutions including a ~1/3 enhancement to approximately account for the so-called Thouless-Valatin correction (i.e. the self-consistence effect for the time-odd part of the 1-body density (see J. Libert et al., Phys. Rev. C60 (1999) 054301)

11 nuclei from ^{156}Sm to ^{174}W (loosely called « rare-earth nuclei »)
8 actinide nuclei from ^{234}U to ^{256}Fm

3 Skyrme interactions SIII, SkM* and Sly4 in use

Moments of inertia rms deviation with data (in units of $\hbar^2$ MeV^{-1})

	SIII	SkM*	SLy4
Rare earth	1.769	2.706	2.940
Actinide	4.582	3.394	3.498
	2.454	1.829	1.885

Corrected for comparison with « rare-earths »
by a factor $(169/245)^{5/3}$

Typical values
35 « rare-earth », 65 actinides

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Phys. Rev. C110 (2024) 024311

Results for odd-even mass differences of well and rigidly deformed odd-even and even-odd nuclei

The Skyrme SIII interaction is in use

We always consider the experimental $I^\pi = K^\pi$ configurations
(no problem with $1/2^\pi$ cases the decoupling constant being always in the « safe » region)

16 odd-N even-Z « rare-earth nuclei » from ^{157}Sm to ^{181}Hf
- 10 config. assigned, 9 obtained correctly
- 3 config. suggested, 2 confirmed
- 1 config. not assigned in ^{165}Gd ($7/2^-$ proposed)
- in ^{165}Dy and ^{171}Yb a ground and isomeric states are found within 108 keV and 95 keV, we found them in the wrong order with an energy error of 156 keV and 168 kev respectively

13 even-N Odd-Z rare-earth nuclei from ^{157}Eu to ^{179}Lu
- 9 config. assigned, 8 obtained correctly
- 3 config. suggested, 3 confirmed
- 1 config. not assigned in ^{161}Eu ($5/2^-$ proposed)

The rms deviation from data for the three-point odd-even mass differences is

For odd-neutron nuclei   78 keV

For odd-proton nuclei   182 keV

T.V. Nhan Hao, N.N. Bao Nguyen, D. Quang Tam, P. Quentin, L. Bonneau, Meng-Hock Koh, submitted for publication at Chin. Phys. C

A point of comparison

In the paper by M.N. Nor, N.-A. Rezle, K.-W. Kelvin Lee, M.-H. Koh, L. Bonneau and P. Quentin, Phys. Rev. C99 (2019) 064306
two separate fits of the average pairing matrix elements within a sample of well and rigidly deformed « rare-earth » nuclei
on either the moments of inertia or the odd-even mass diffrerences
using the SIII iteraction had resulted in similar results for the matrix elements

Comparing the qualities of these separate fits supposedly more apt to reproduce each of the data with the current approach should provide a further test of its relevance

MOMENTS OF INERTIA
rms deviation with dat
in $\hbar^2$ MeV^{-1}

Separate fit	Our calc.
1.75	1.77

ODD-EVEN MASS DIFFERENCES
rms deviation with data
in keV

Separate fit neutron	Our calc. neutron	Separate fit proton	Our calc. proton
87	78	172	182

SOME CONCLUDING REMARKS

Our approach is not directly a fit
Our approach does not provide an interaction
It provides a value of average pairing matrix elements for each considered ground state

In principle there is no such thing as an universal residual interaction since it depends on the mean field by definition

However to go further we cannot in fact avoid fitting an interaction taking stock of the present study

Our current approach suffer from two limitations

- It is limited by the seniority force ansatz (no state dependence of the matrix elements)

- It is restricted a priori to ground states of well and rigidly deformed nuclei (because only there we have relatively safe handles on relevant data)

Thus to extend to other nuclei and other states (potential energy surfaces, fission barriers etc.) we need to define through fits in a large enough region, the intensity parameters of an interaction to communicate there the information on pairing correlations gained where it was possible to extract them from data

This is currently undertaken